4-Phenyltoluene
644-08-6 | DTXSID4047177

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 1.71e-02 mmHg

Global applicability domain: Inside

Local applicability domain index: 7.29e-01

Confidence level: 8.04e-01

Nearest Neighbors from the Training Set

Image not found
1,2-Dinitrobenzene
Measured: 1.31e-02
Predicted: 1.59e-04

Image not found
2-Methylnaphthalene
Measured: 1.22e-02
Predicted: 2.48e-02

Image not found
5-Aminoquinoline
Measured: 1.42e-02
Predicted: 1.66e-04

Image not found
Heptylbenzene
Measured: 2.52e-02
Predicted: 2.77e-02

Image not found
2-Propenoic acid, propyl ester
Measured: 3.16e-02
Predicted: 16.8